Phase retrieval from non-periodic images in the presence of vortices

The research material presented in this talk is the work of :

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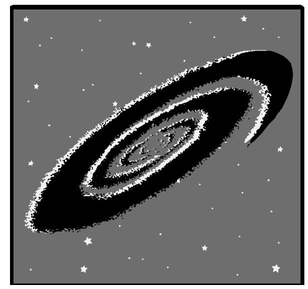
Vortices

- Appear everywhere in nature
  - whirlpools
  - spiral galaxies
  - combustion engines
  - screw dislocations in crystals



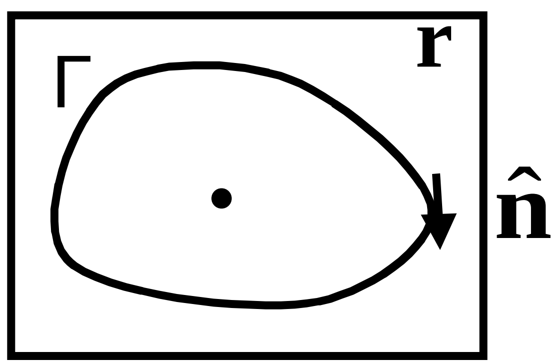
- Are important in quantum mechanics
  - superfluids
  - superconductors
  - Bose-Einstein condensates
- Are important in visible-light optics
  - diffraction free vortex beams
  - vortex solitons
  - holographically produced screw dislocations
- Occur often in electron microscopy

What is a vortex?

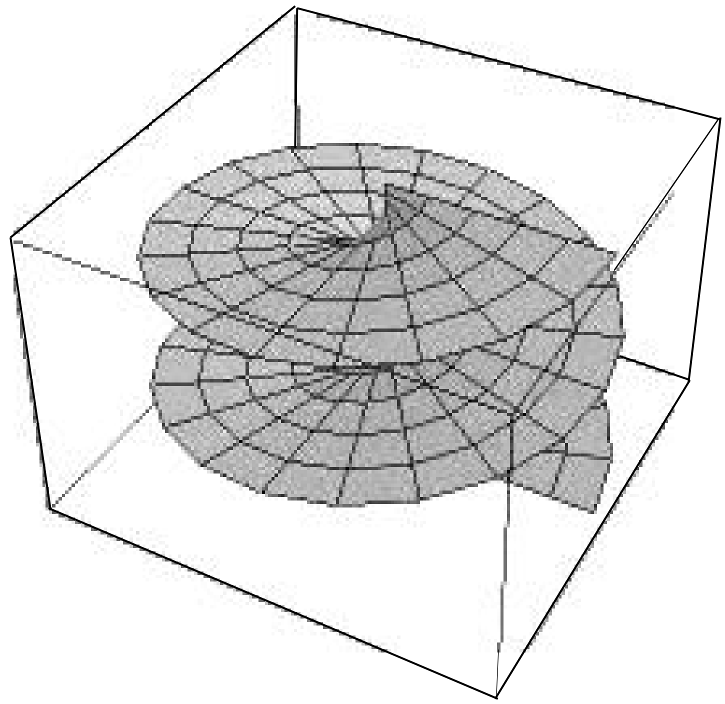
- A discontinuity in the phase of a wavefunction
- $\Psi(\mathbf{r}) = |\Psi(\mathbf{r})|e^{i\theta(\mathbf{r})}$
- Wavefunction $\Psi(\mathbf{r})$ is continuous and single valued
- Probability density (intensity) of the wavefunction, $|\Psi|^2$ is continuous and single valued
- However, if $|\Psi|^2 = 0$, then the phase is not well defined
- Thus phase can be discontinuous or multivalued

Circulation of the phase

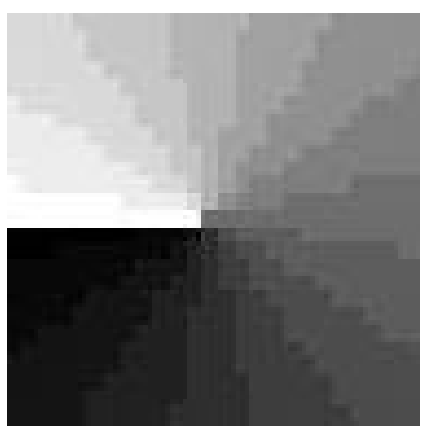
- Phase is defined modulo 2π
- Circulation of the phase is not necessarily zero
- ie $\oint_{\Gamma} \theta(\mathbf{r})\,?\,d\hat{\mathbf{n}} = 2\pi m$



- Γ is closed path of loop integral
- $\hat{\mathbf{n}}$ is unit vector tangential to the path
- *m* is integer “topological charge”
- if $m \neq 0$ there exists a vortex with its core located inside the path Γ



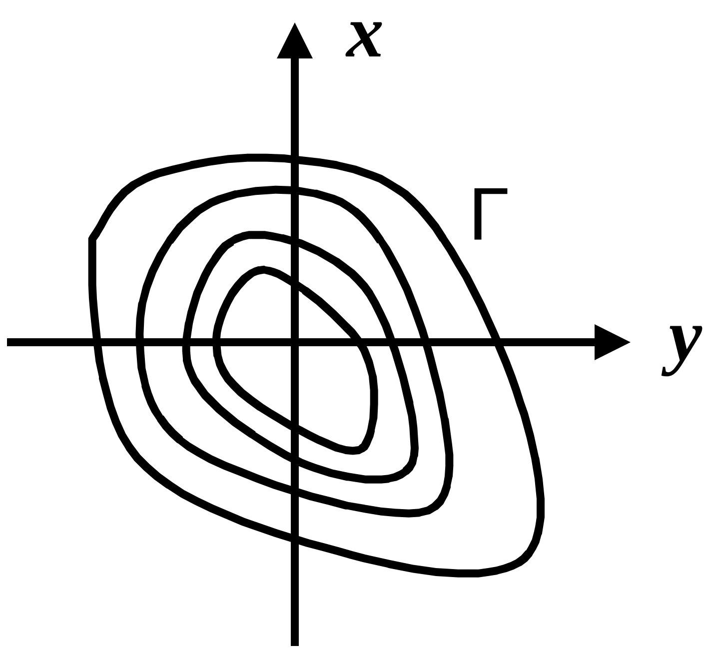
- Phase behaviour about vortex core with topological charge 1
- Note “spiral staircase” structure



- Vortex shown in greyscale map of phase
  - white corresponds to phase π
  - black corresponds to phase $-\pi$

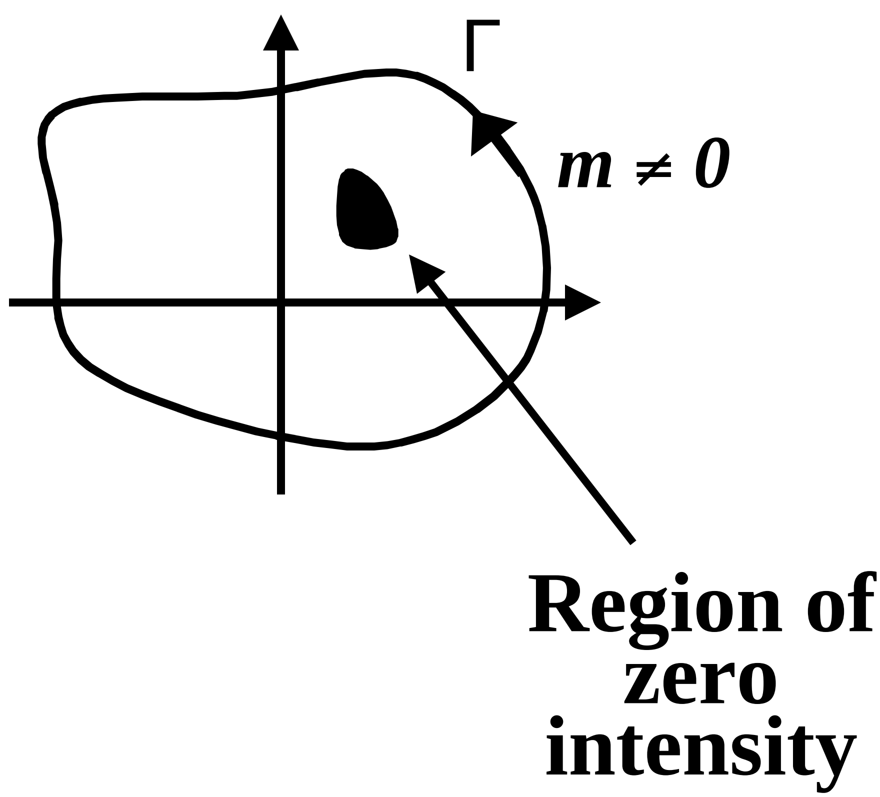
Theorem 1

- The same circulation will be possessed by all loops Γ in the parameter space **r** which can be continuously deformed into each other without encountering any zeros of the field.



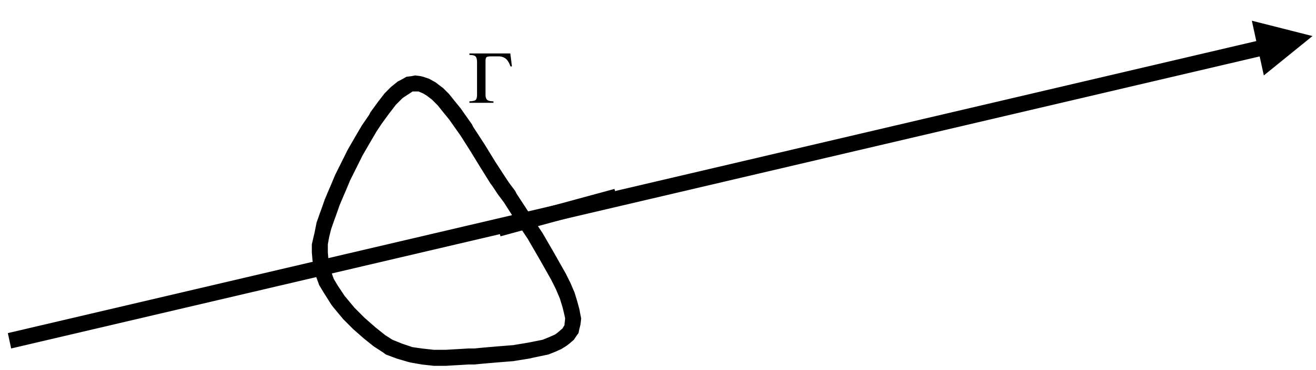
Theorem 2

- If a loop has nonzero circulation, it must enclose a point/region of zero intensity
- Hence vortices are associated with zeros of intensity

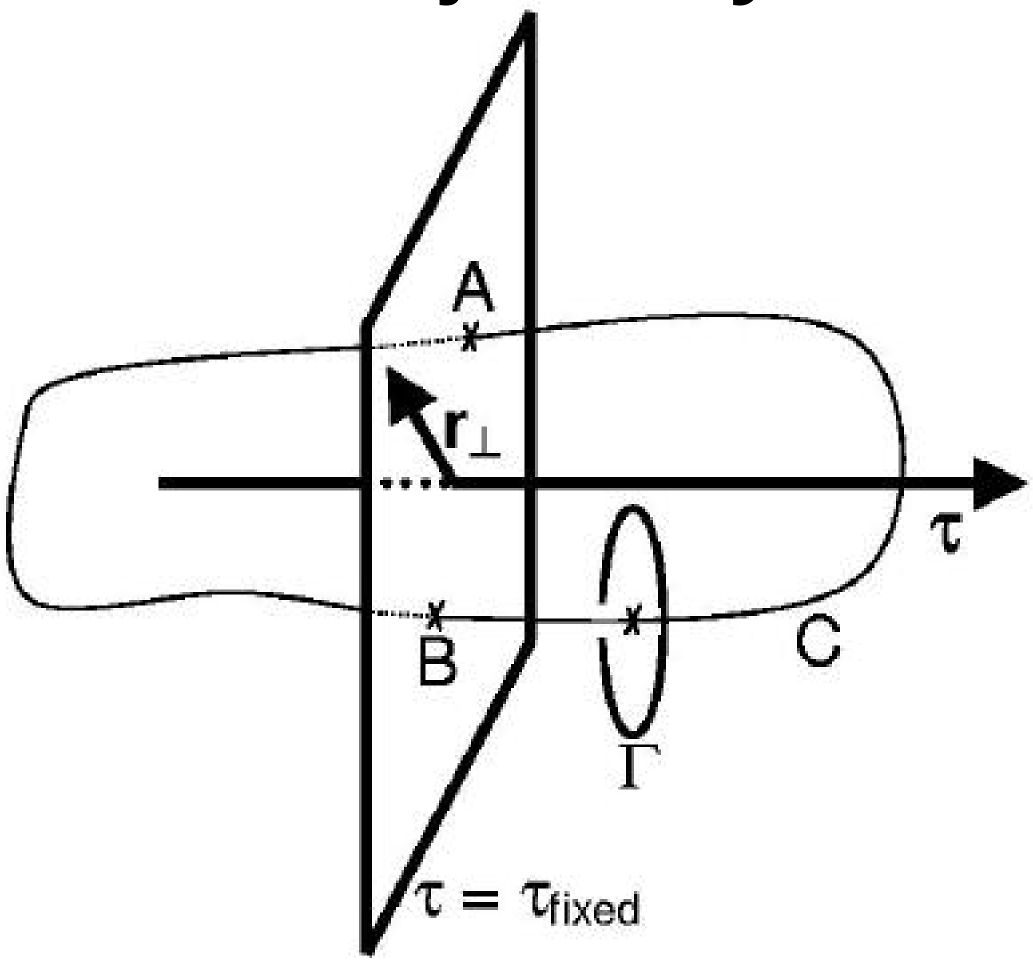


Theorem 3

- The region over which the intensity is zero is either an infinite line or a loop in the parameter space **r**.
  This line or loop is a
  Vortex Trajectory
- This is an immediate consequence of Theorem 2 - the path Γ cannot “unstring” itself from the zero region containing the trajectory.



Example vortex trajectory

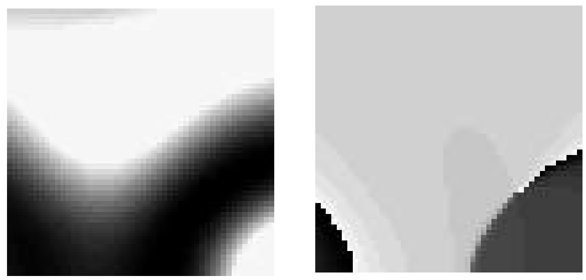


- Vortex trajectory C cuts plane at points A and B, where counter-propagating vortices exist in plane.
- Path Γ cannot be removed from trajectory loop, and has constant circulation, regardless of its location.

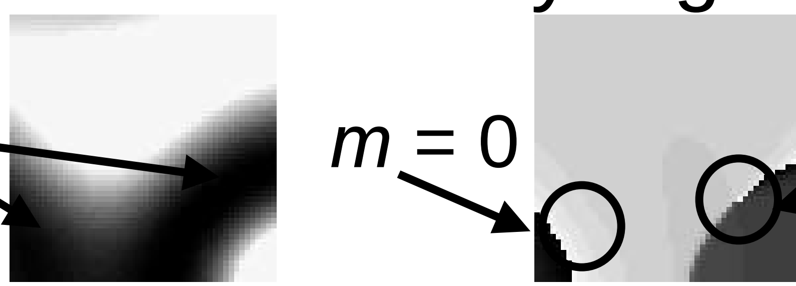
- The same vortex will have a different direction of rotation depending on the observer’s vantage point.
- One trajectory may result in many vortices being observed in a given plane.
- They will have related charges and directions of rotation
- Thus it is more useful to consider the behaviour of vortex trajectories rather than individual vortices in a plane.

Tracking vortex trajectories

- Compute wavefunction in 2D plane.

Intensity  Phase

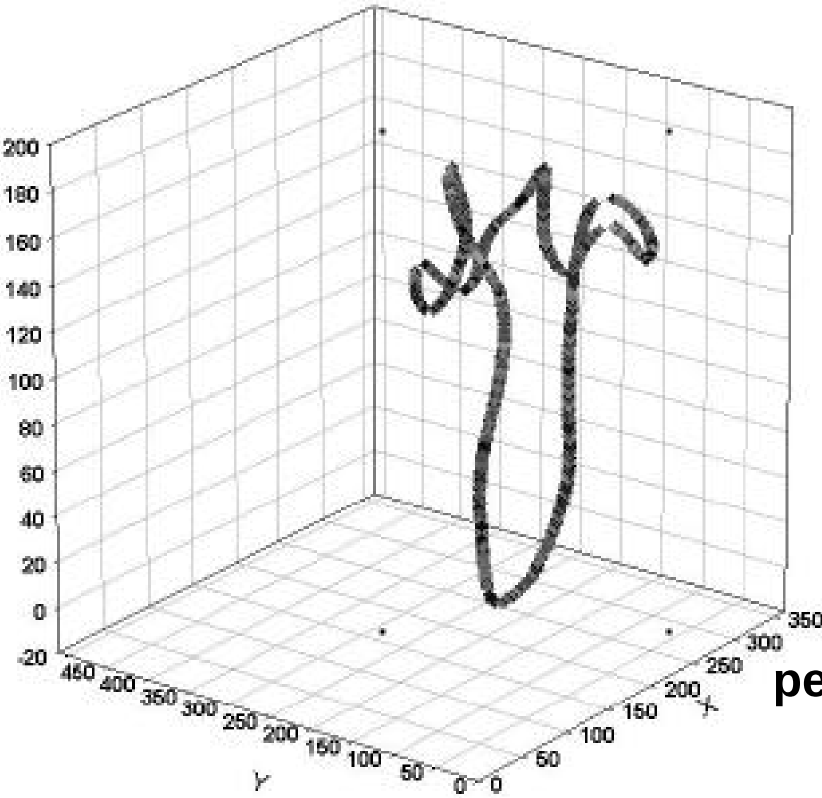
- Locate zeros of intensity.
- Compute circulation of phase around zero intensity regions.



- If circulation clearly non-zero (ie |*m*| >δ), designate zero point as part of a vortex trajectory.
- Repeat this process for many planes throughout parameter space

Calculated vortex trajectory

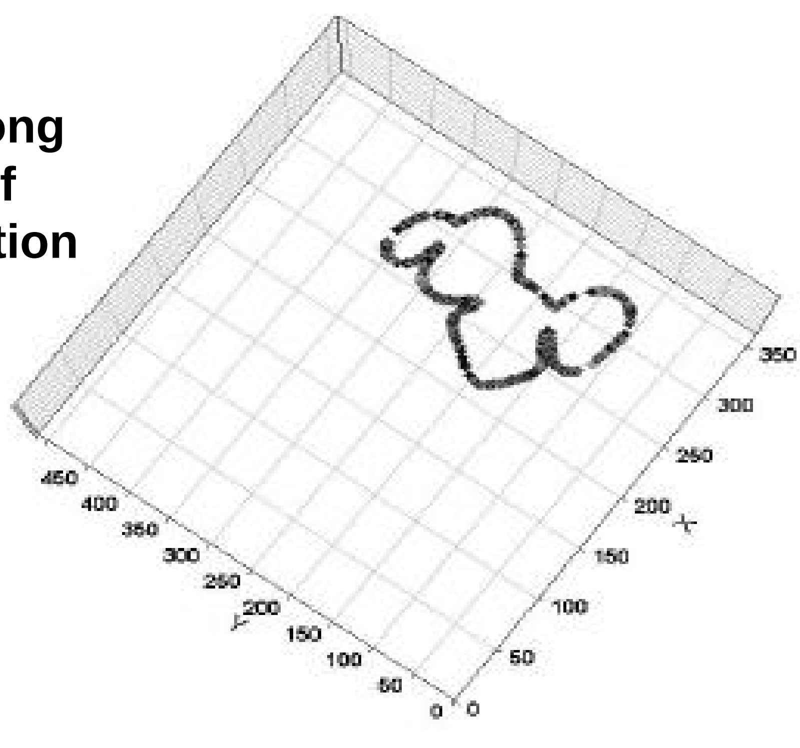
defocus



(x,y) plane perpendicular to direction of propagation

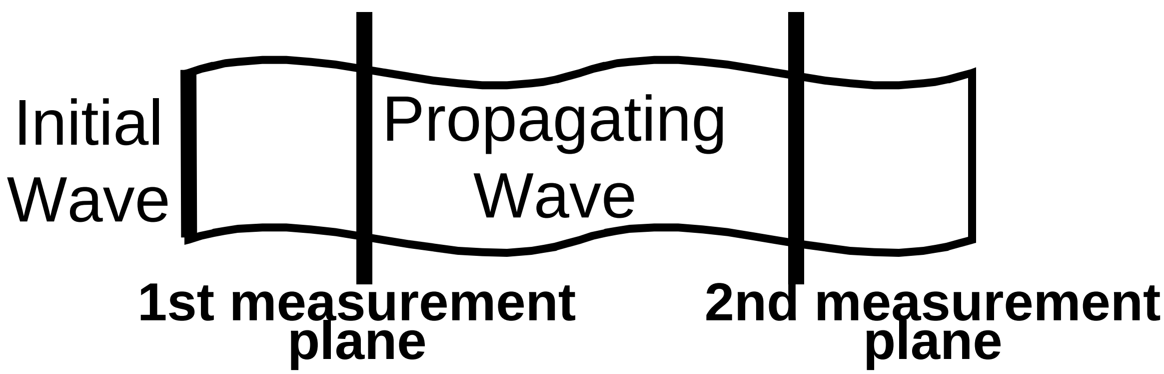
Vortex trajectory for a model wavefunction propagating in space

View along axis of propagation



Phase retrieval and vortices

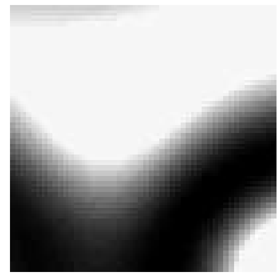
- The phase of a wavefunction is important information
- It can't be measured directly
- Non-interferometric methods require multiple measurements, usually in more than one plane



- Vortices may occur in one or more planes of measurement

- A vortex requires a region of zero intensity to exist
- Phase retrieval methods which assume intensity is non-zero everywhere therefore assume that there are no vortices.
- Such methods can’t retrieve phase correctly when vortices are present.
- This is a known problem with methods such as those based on flux continuity (solving the Transport of Intensity Equation).
- We look for a method which bypasses this problem.

- General phase retrieval methods must assume that
  - intensity may be zero
  - phase may be discontinuous.



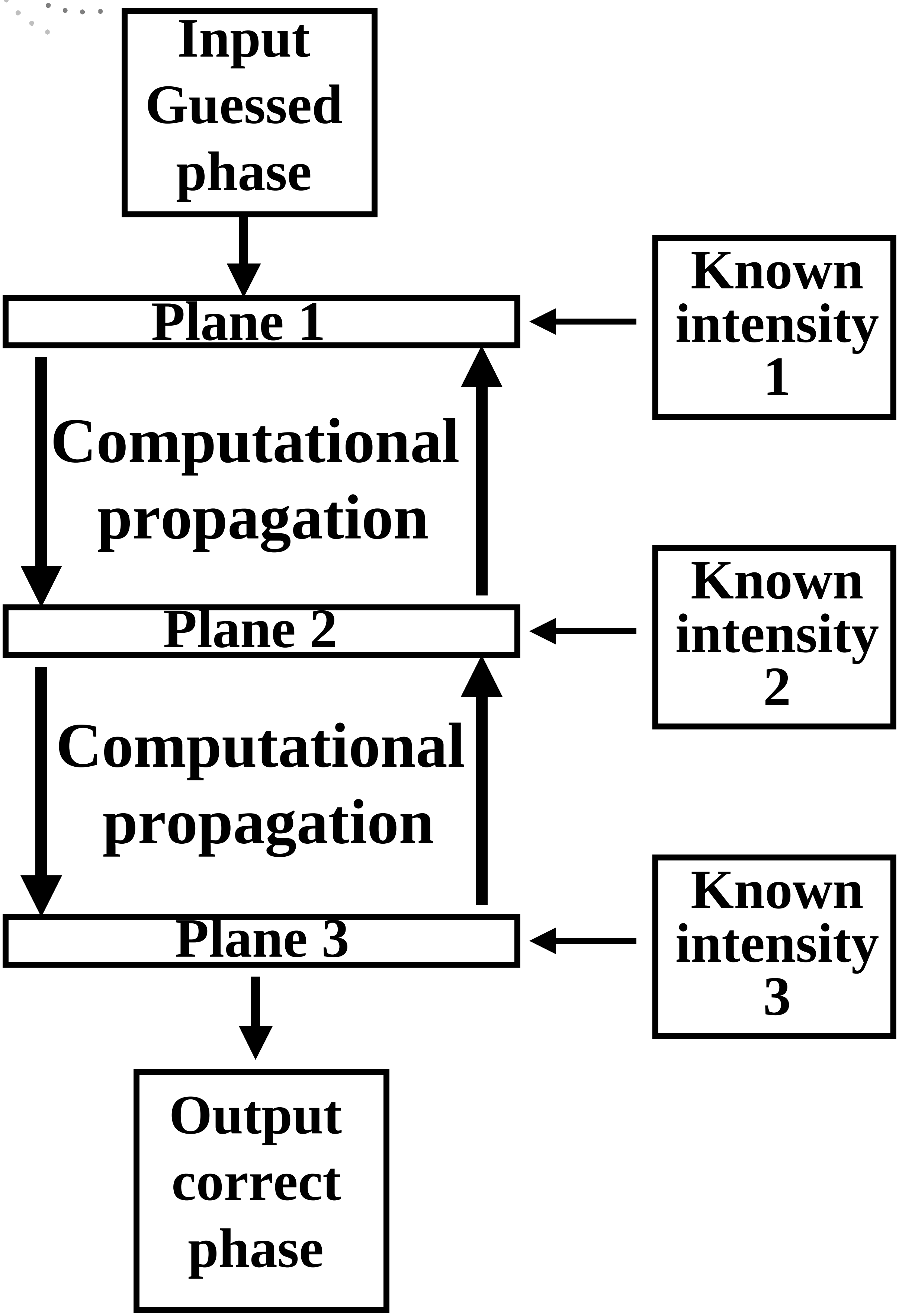
- Note that the wavefunction remains continuous, even if phase discontinuities exist.
- It makes sense to find a method which deals with the entire wavefunction.
- It does not make any particular assumptions about phase continuity.

- We propose an iterative method which uses a through focal series of images as input.
- Images measured in 3 or more planes are required.
- The algorithm is that suggested by Saxton (1978) for two image planes.
- Uniqueness issues are discussed in:
  - L. J. Allen, H. M. L. Faulkner, K. A. Nugent, M. P. Oxley and D. Paganin, Phys Rev E, **63**, 037602 (4 pages).

Outline of algorithm

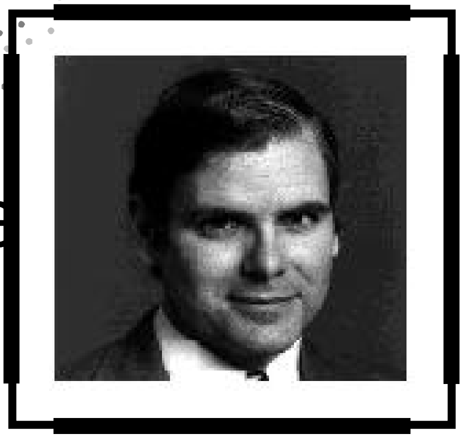
- Given initial measured intensity in one plane, guess the phase in that plane
- Computationally propagate wavefunction to next plane. Since wavefunction is continuous, propagation produces no problems.
- If new intensity is incorrect, correct it and propagate back, or forward to next plane
- Error in calculated wavefunction will decrease
- Repeat until propagated intensity is correct

Through Focal Series Method



Data used

Image

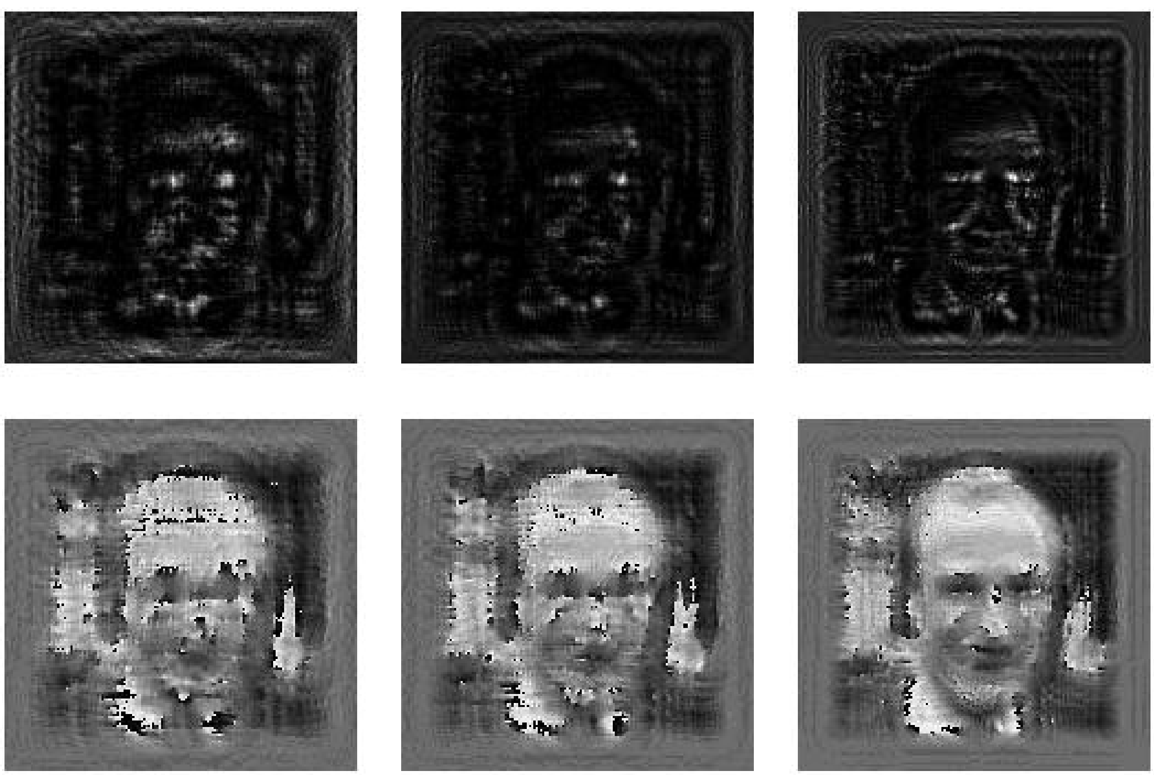


Phase

- 80keV electrons used with 75Å, image size (equivalent to 1.14mm image for 6328Å HeNe laser).
- Initial image and phase are propagated in space to give a through focal series in 3 planes.

Image

Phase



-750Å (-11.37mm) | -500Å (-7.58mm) | -250Å (-3.79mm)

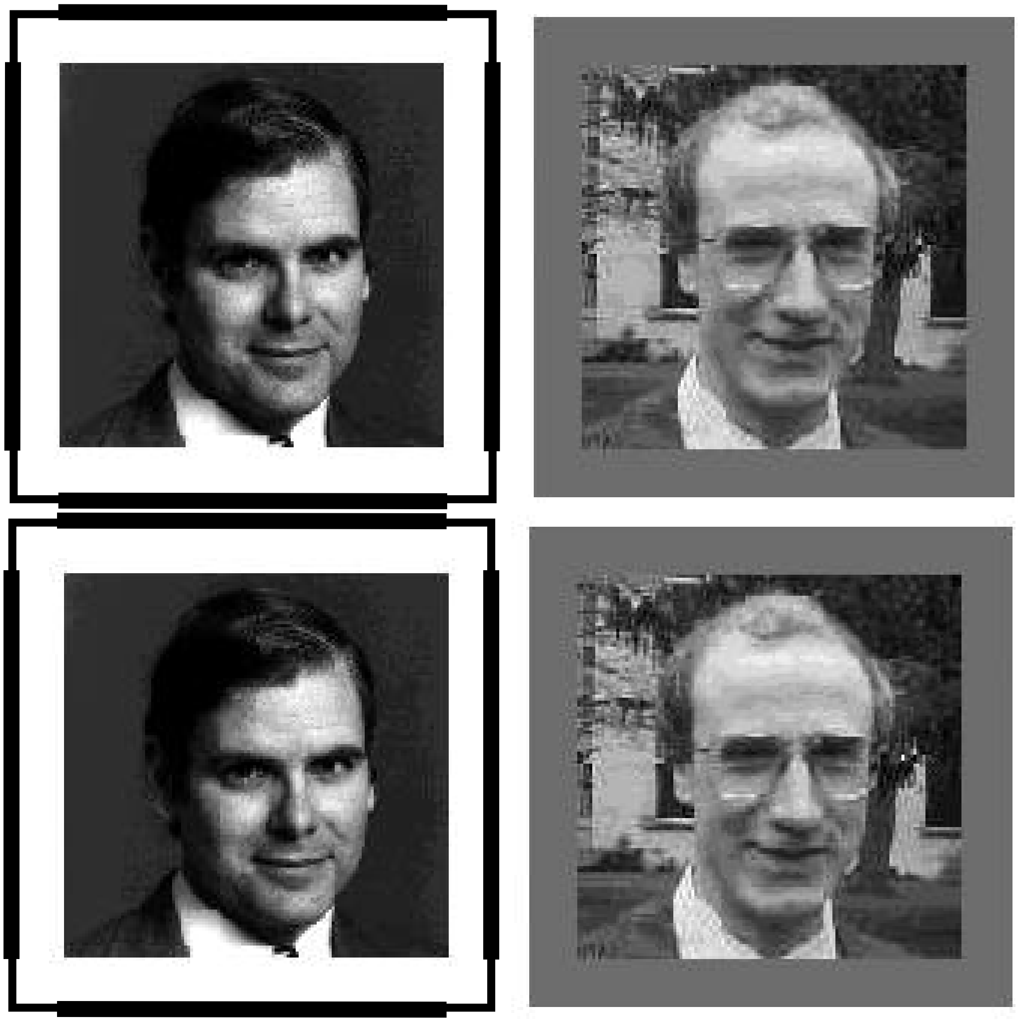
- Note that vortices exist in the phase in every plane of TFS.
- Our aim is to

  1) Find phase at each TFS plane

  2) Propagate phased wavefunction back to original data plane, for comparision with input images.

Results

Image Phase



Initial data

Retrieved results

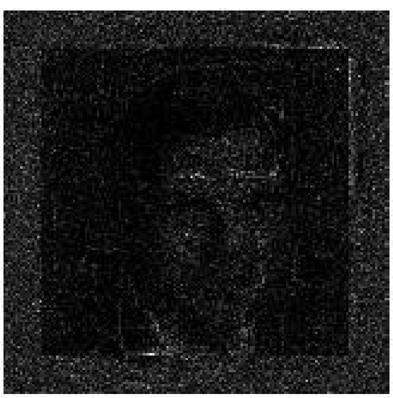
- Retrieved phase after 1500 iterations has sum squared error of 3.046×10^{-11}.
- Method has successfully coped with vortices in the phases of the through focal series.

Results when image data is noisy

Image Phase

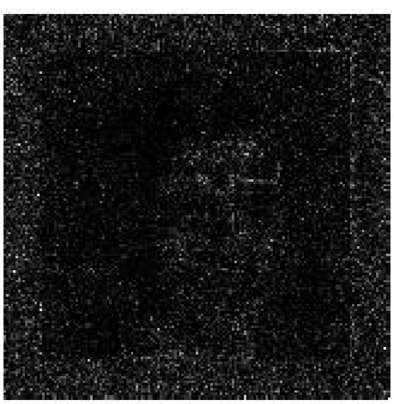
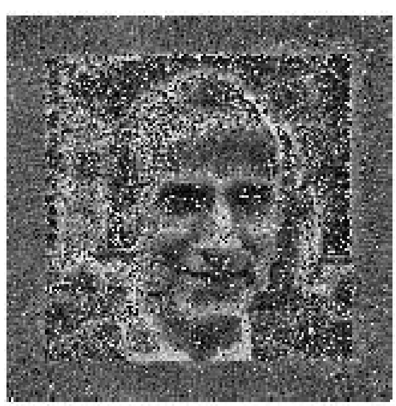

≥ 10% noise

SSE ≈ $3\text{x}10^{-3}$




≥ 20% noise

SSE ≈ $1\text{x}10^{-2}$

≥ 30% noise

SSE ≈ $2\text{x}10^{-2}$

Conclusion

- Vortices are so common they must be allowed for in many phase retrieval situations.
- This requires allowing the phase to be discontinuous, and the intensity to be zero.
- The iterative retrieval method accurately retrieves phase in the presence of vortices.
- It is effective with noisy data and numerically robust.
- It can include correction for known microscope aberrations.
- It is applicable to a large number of physical situations.